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TECHNICAL MEMORANDUM No. 8/M/51

Calculation of the Explosive Power of Mixtures of Chlorine Trifluoride and Ammonia (Both Liquid)

G. H. S. Young

Incl #1
ORD-TR 8AT-329

Waltham Abbey
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SUBJECT: Calculation of the Explosive Power of Mixtures of Chlorine Trifluoride and Ammonia (Both Liquid)

TO: The Chief of Ordnance
Department of the Army
Washington 25, D.C.

Attn: ORDGU-IN

1. Reference - None

2. Forwarded herewith as Inclosure #1 is E.R.D.E. (Explosives Research & Development Establishment) Technical Memorandum No. 8/M/51 entitled "Calculation of the Explosive Power of Mixtures of Chlorine Trifluoride and Ammonia (Both Liquid)", dated July 1951.

3. Abdract of the Report is as follows:-

The explosive power of mixtures of Liquid NH_3 and ClF_3 within the range of ratios of 1.4 to 2.3 moles of NH_3 per mole ClF_3 are calculated. Calculations are based on the correlation of the Berthelot Product for the mixtures to its value for Picric Acid under normal condition in the explosive calorimeter. The optimum mixture of 2.8 parts by weight of ClF_3 with 1 part of NH_3 gave a calculated value of 188 which is theoretically about equivalent to Methyl Nitrate (185) and somewhat better than RDX (168). These calculations assume intimate mixture and complete reaction which would be very difficult to achieve in practice.

(Trip)

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No. 8/M/51

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by

G.H.S. Young

This memorandum does not contain classified information of overseas origin.

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Reference: XR 880/12.

1. INTRODUCTION.

The explosive effectiveness of a given substance relative to that of the accepted standard, picric acid, as measured for example by the Trautzl Block or the Ballistic Mortar methods, is found to be fairly well correlated with the relative value of the "Berthelot Product". The latter is proportional to nQ, where Q is the heat (per gm) which would be liberated by the chemical change which actually takes place in the explosion, if it could take place in the same way at ambient temperature (300°K.), while n is the number of gram molecules of gaseous products obtained in the explosion from one gram of the substance. The Explosive Power (Pr) is therefore defined as one hundred times the ratio of the value of this Berthelot Product for the given substance under stated conditions to its value for Picric Acid under normal conditions in the explosive calorimeter.

2. SYSTEM CONSIDERED.

Assuming approximate thermodynamic equilibrium the principal reaction within the range of mixture ratios studied (1.4 to 2.3 moles. of NH_3 per mole of ClF_3) is as follows:-

$$ClF_3 + x\,NH_3 = 3HF + HCl + \frac{x}{2}N_2 + \left(\frac{3x}{2} - 2\right)H_2$$

As x approaches the boundary value $\frac{4}{3}$, the temperature of the adiabatic constant volume flame rises steeply (see Fig.2) and the dissociation products, atomic chlorine and atomic fluorine become appreciable in amount (3-4%), the amounts of the molecular forms, Cl_2 and F_2, being somewhat less while the dissociation of hydrogen and nitrogen remains effectively small at the high pressures involved.

The main reaction alters in two stages as x is still further diminished; the hydrogen virtually disappears and atomic chlorine and (ultimately) fluorine appear as main products.

The necessary thermodynamic data for calculating the flame temperature and explosive power at these lower values of x can only be estimated rather imperfectly, but fortunately the optimum mixture ratio, as regards explosive power, appears to lie within the higher range of x as indicated by the graph (Fig.1). It was therefore not necessary to investigate the lower range of x in detail.

The heat of formation of gaseous ClF_3, about which there has been some variation of opinion, was taken to be 28 k.cal. per mole (H.V. v. Wartenberg, Z.anorg.Chem.,1949, 258, 356) and the latent heat of vaporisation as 5.k.cal. per mole. The remaining thermodynamic data was obtained from Pike's tables and from the compilation of the American Bureau of Standards.

The volume of the system was taken to be the sum of the volumes of the liquid components ClF_3 and NH_3 at 300°K. (assumed to be under suitable pressures).

/3.RESULTS.

3. RESULTS.

The essential results of the calculations are as follows :-

Temperature °K.	x	Pr.
3870	2.24	186.55
4065	2.07	187.7
4355	1.85	187.76
4455	1.78	187.65
4645	1.65	187.3
4840	1.51	186.2
4935	1.42	184.6

The decimal places in the value of Pr are of little significance except in showing the smooth trend of the calculated values, with a definite maximum of about 188 at $x = 1.95$.

This maximum figure, 188, for a mixture of 2.8 parts by weight of ClF_3 with 1 part of NH_3, can be compared with:

Explosive	Pr.
Picric Acid	100
T.N.T.	108
R.D.X.	168
Methyl Nitrate	185
Nitromethane	154

Thus the optimum mixture is theoretically about equivalent to methyl nitrate in explosive power and somewhat better than R.D.X.

It seems apparent from these calculations that liquid fluorine would give a higher explosive power with liquid ammonia, because the energy per unit mass is greater, and there would be no heat of formation term to be taken into account.

The calculations assume that it would be possible to get an intimate mixture, and complete reaction. In practice this would be very difficult to achieve, and explosion rather than detonation, might occur.

4. ACKNOWLEDGMENTS.

The calculations on which this note is based were carried out by Dr. B.M. Cavanagh and Miss M.A. Hooper.

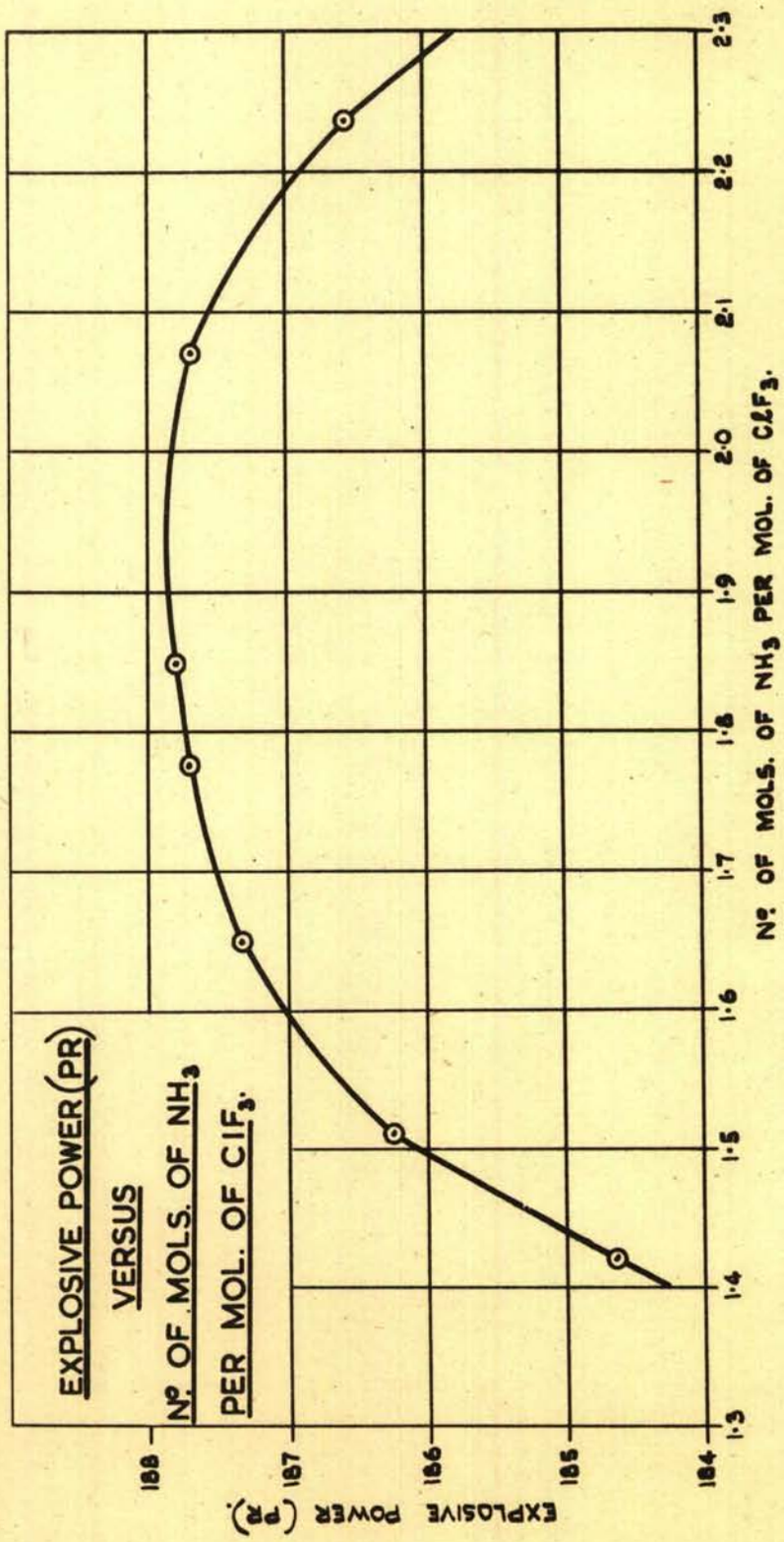

FIG. I.

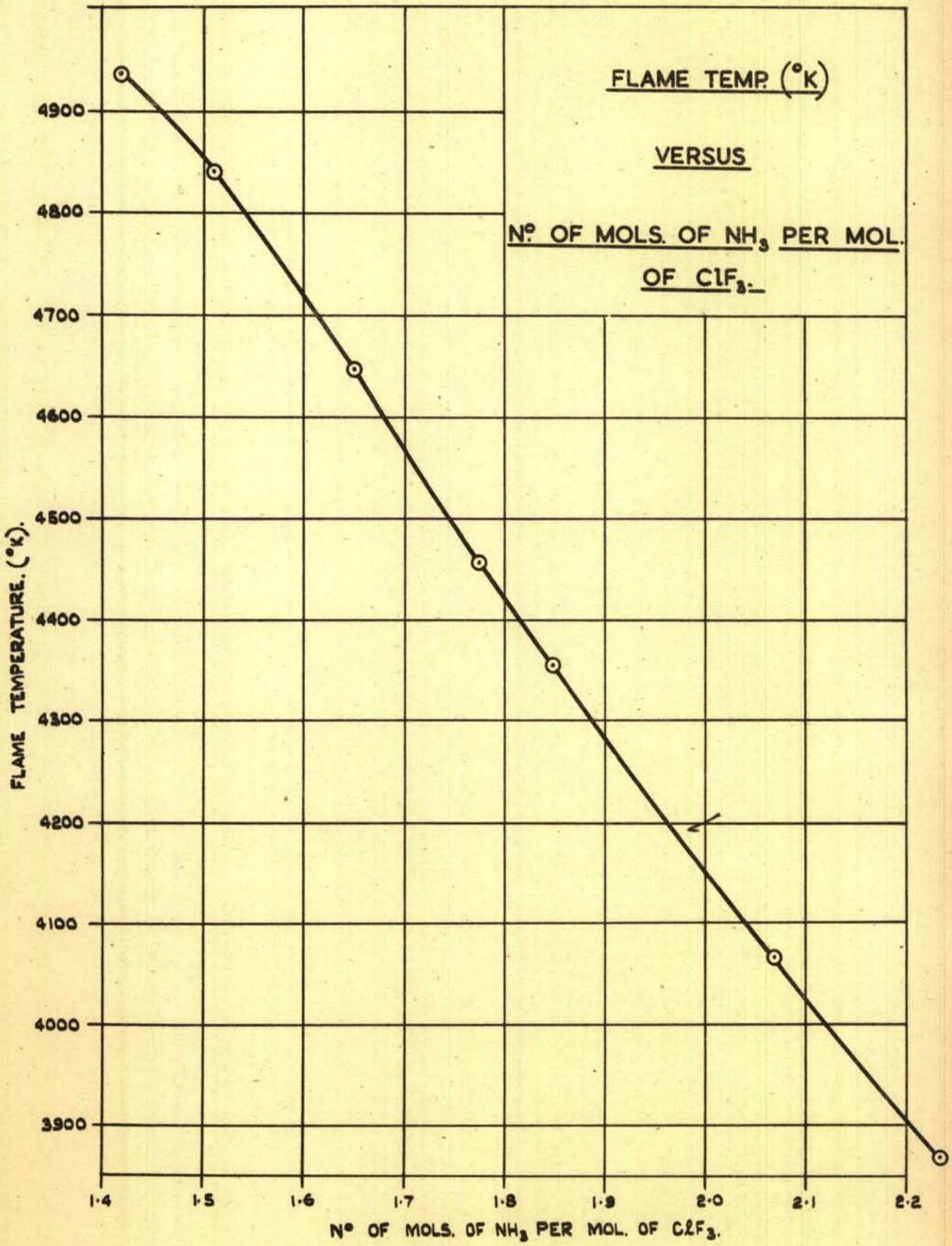
FLAME TEMP. (°K)
VERSUS
Nº OF MOLS. OF NH3 PER MOL. OF ClF3.
FLAME TEMPERATURE. (°K).
4900
4800
4700
4600
4500
4400
4300
4200
4100
4000
3900
1·4
1·5
1·6
1·7
1·8
1·9
2·0
2·1
2·2
Nº OF MOLS. OF NH3 PER MOL. OF ClF3.

FIG. 2.